

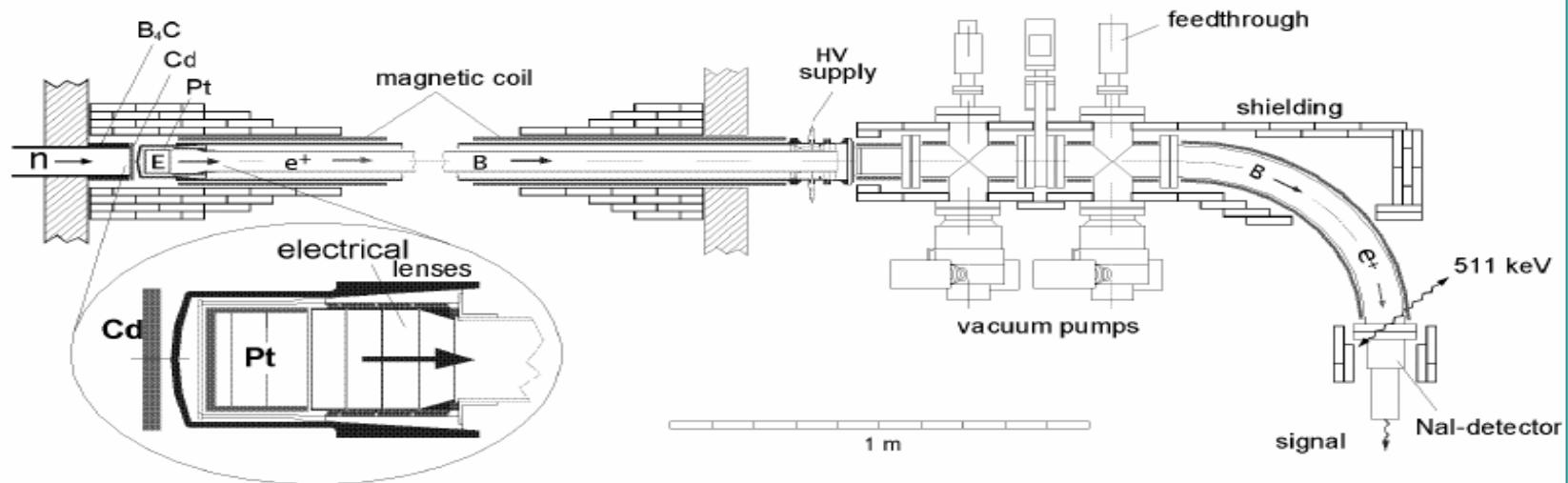
Positron Annihilation Induced Auger and Gamma Spectroscopies of Nanostructures and Surfaces

Alex Weiss

The University of Texas at Arlington

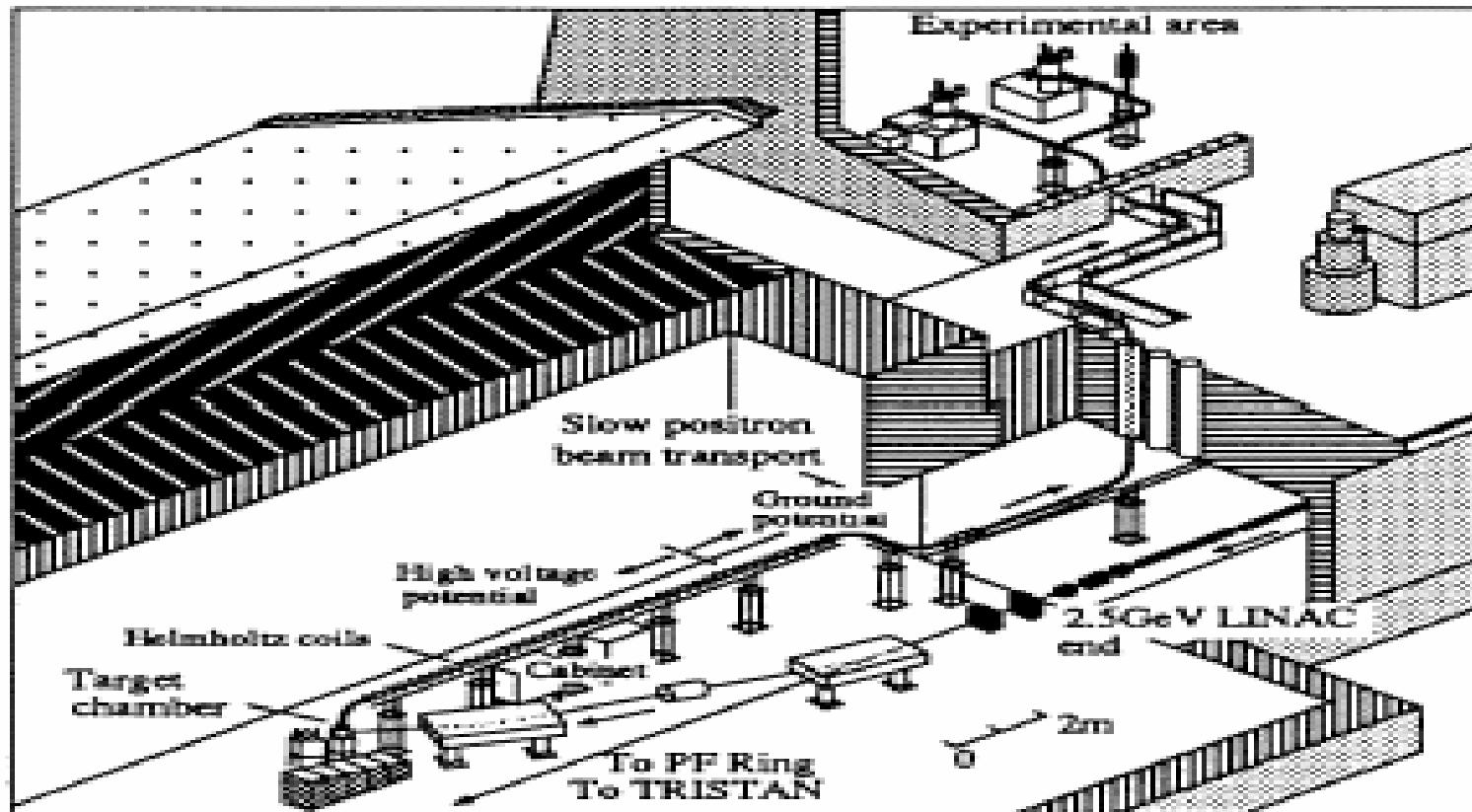
Intense low energy **positron** beams from neutron sources

POSITRON BEAM AT THE NEUTRON GUIDE PF 1 / ILL



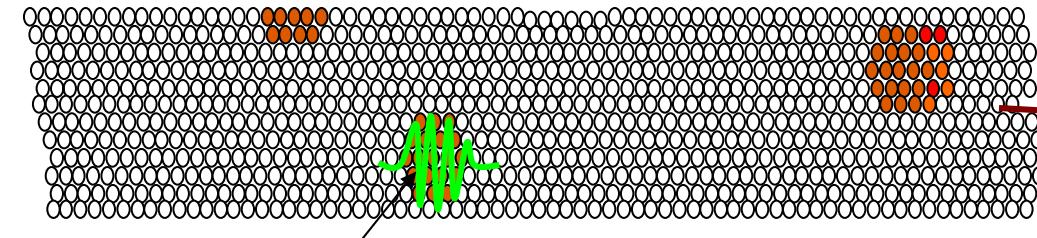
©Christoph Hugenschmidt

Intense positron beams from electron LINACs



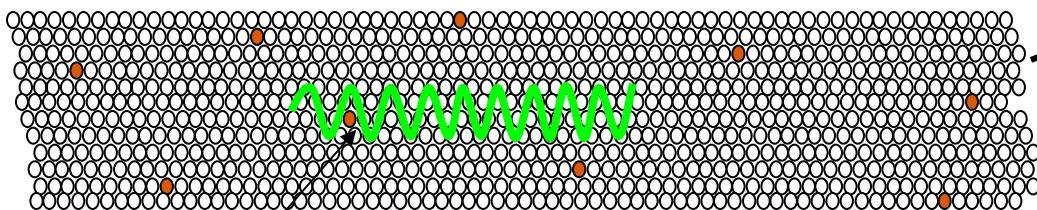
Proposed KEK intense positron beam facility

Schematic diagram of structure of dilute Fe-Cu alloy



Localized positron wave function

Fe-1.0 wt % Cu (2h aged) at 550⁰ C



Delocalized positron wave function

Fe-1.0 wt % Cu (Quenched)



Fe atom
(d ~0.235nm)



Cu atom
(d ~0.256nm)



Cu nano particle
(d ~ 4 nm)

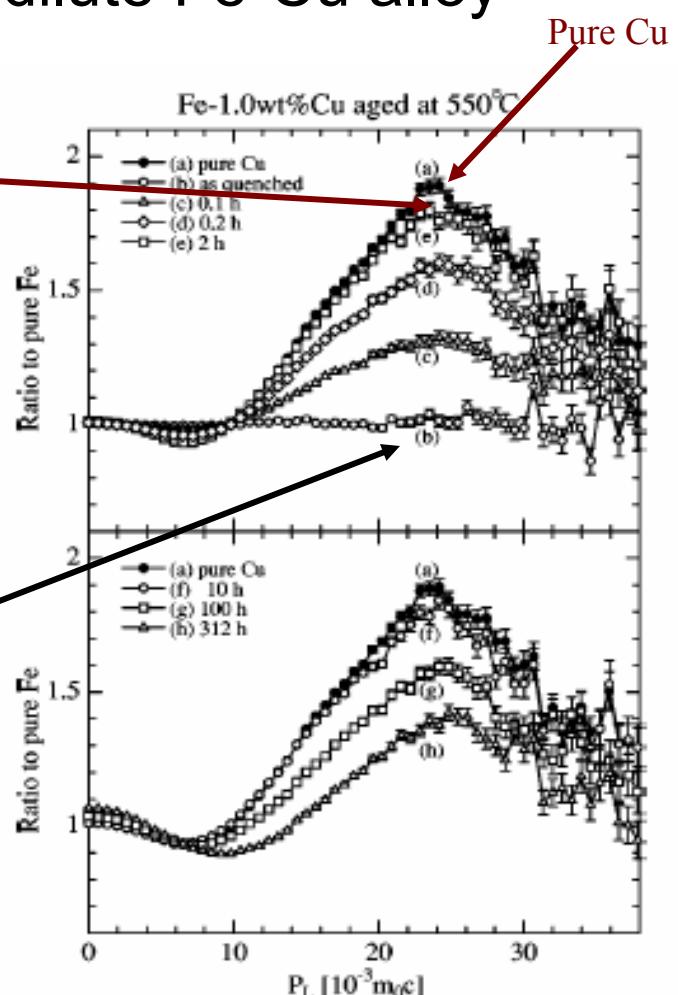
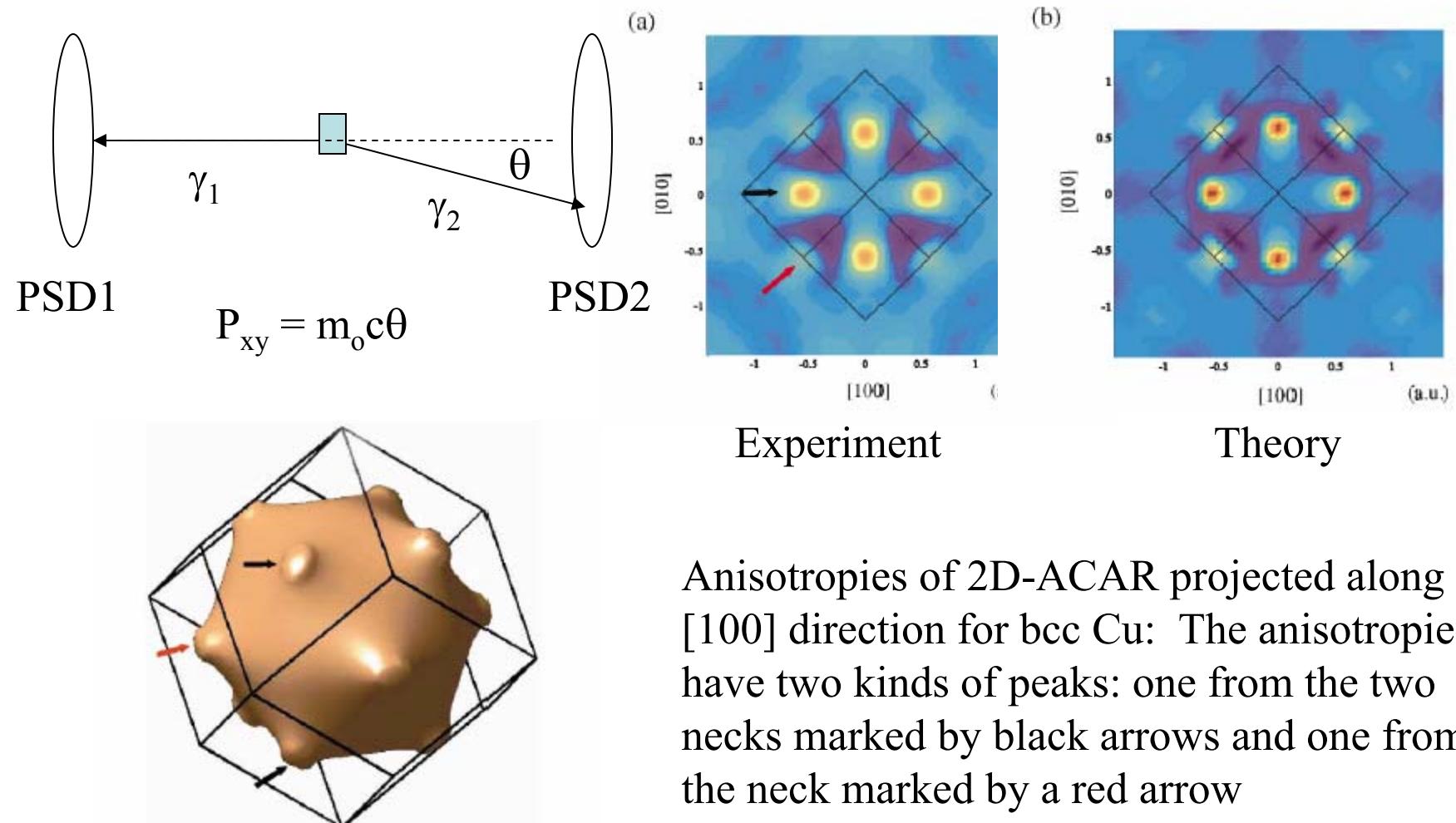
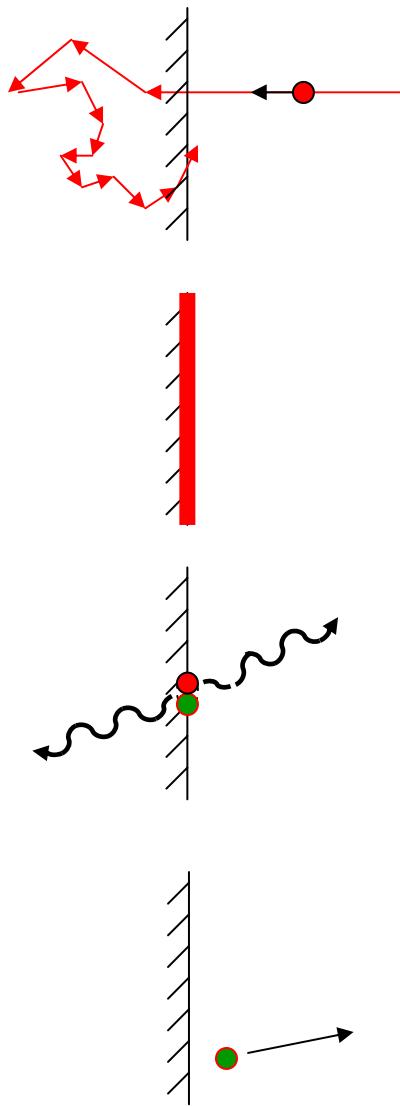


FIG. 3. Ratio curves of the CDB spectra of (a) pure Cu, the Fe-1.0 wt % Cu alloys (b) as quenched, after (c) 0.1 h, (d) 0.2 h, (e) 2 h, (f) 10 h, (g) 100 h, and (h) 312 h aging with respect to that of pure Fe. The shape of the ratio curve is characteristic of each chemical element.

2D-ACAR Measurement of Fermi Surface of BCC Cu Nanoparticle





Low energy (~10ev) positron in.

Implantation, thermalization,
diffusion, encountering the surface

$10^{-12} - 10^{-11}$ sec

Positron trapped in surface state

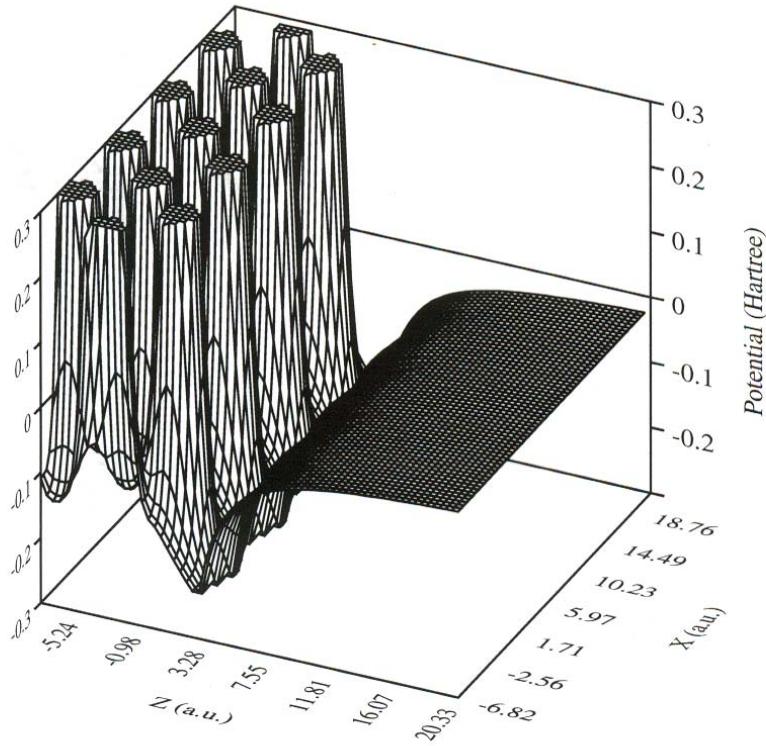
10^{-10} sec

Annihilation of surface state
positron with core electron

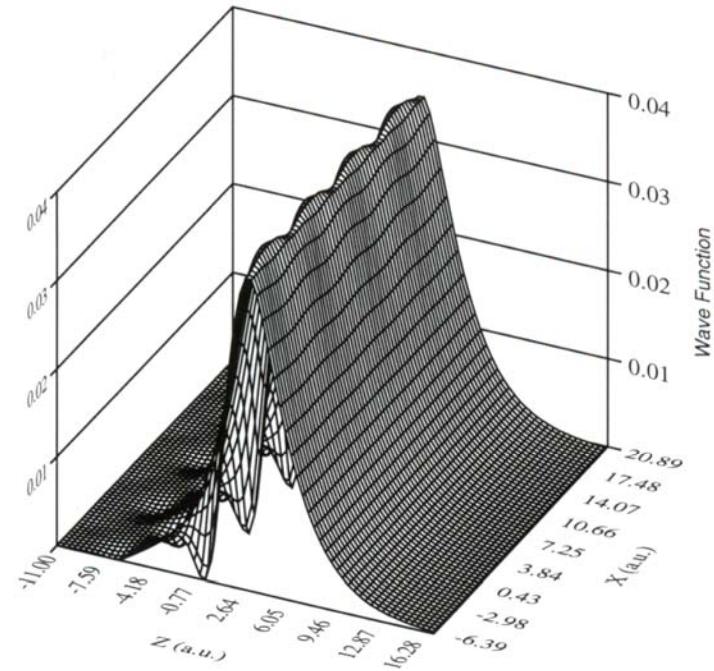
10^{-14} sec

Emission of Auger electron –

**Higher energy (20-800 eV)
electron out.**

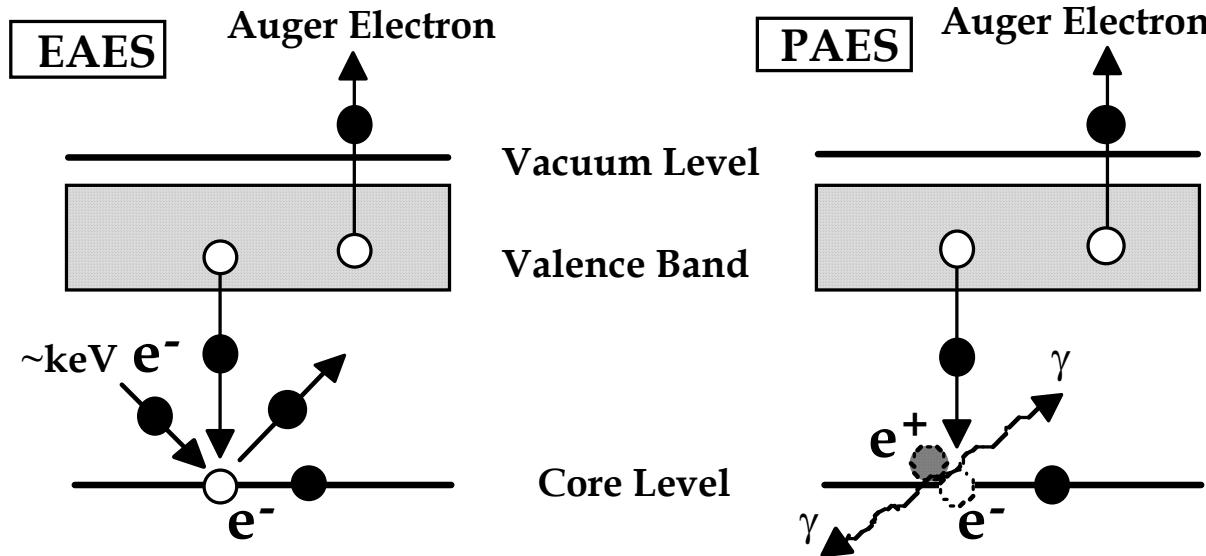


Positron Potential at Cu(100)
surface



Positron-surface-state wave function at
Cu(100) surface

Comparison of core-hole creation mechanism in EAES and PAES



EAES - core electrons are removed by collisions. Incident electron beam energy must exceed the core binding energy.

PAES - core hole created via a matter-antimatter annihilation. Incident positron beam energy can be made arbitrarily low.

Auger transition - the same in both cases.

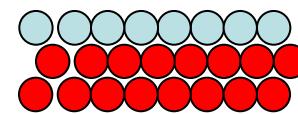
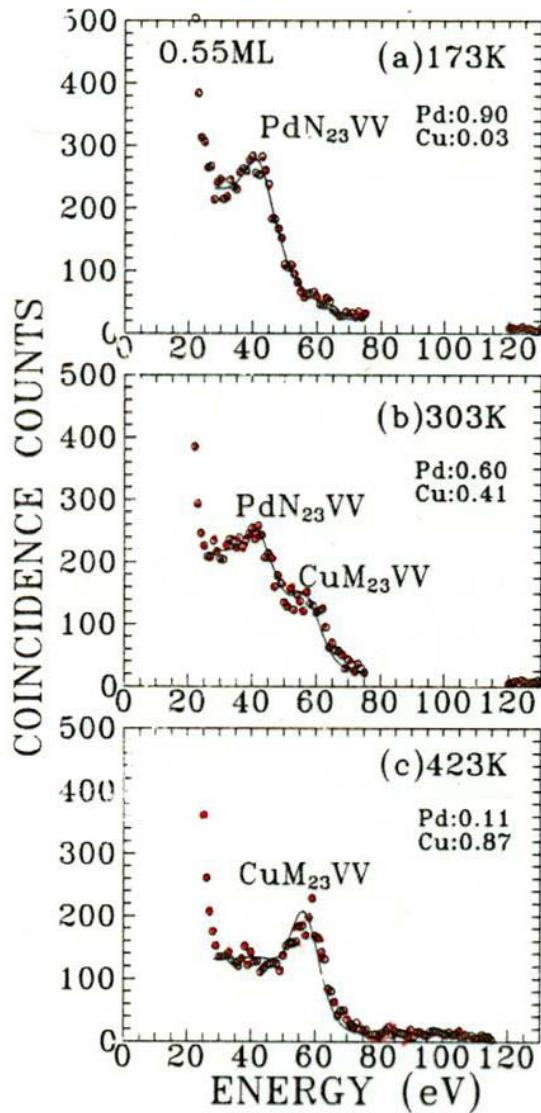
Principal Advantages of PAES:

1. Very low background-elimination of primary beam induced secondary electron background.
2. Higher surface selectivity than other electron spectroscopies.
3. Selective sensitivity to nano structures and impurities.

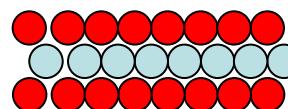
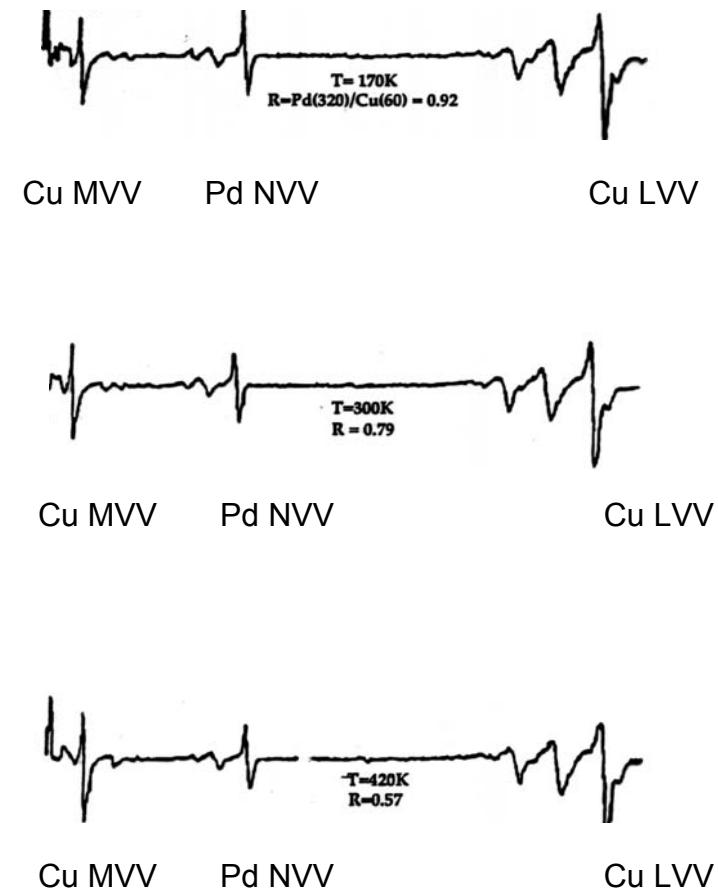
PAES vs EAES

Pd  deposited on Cu 

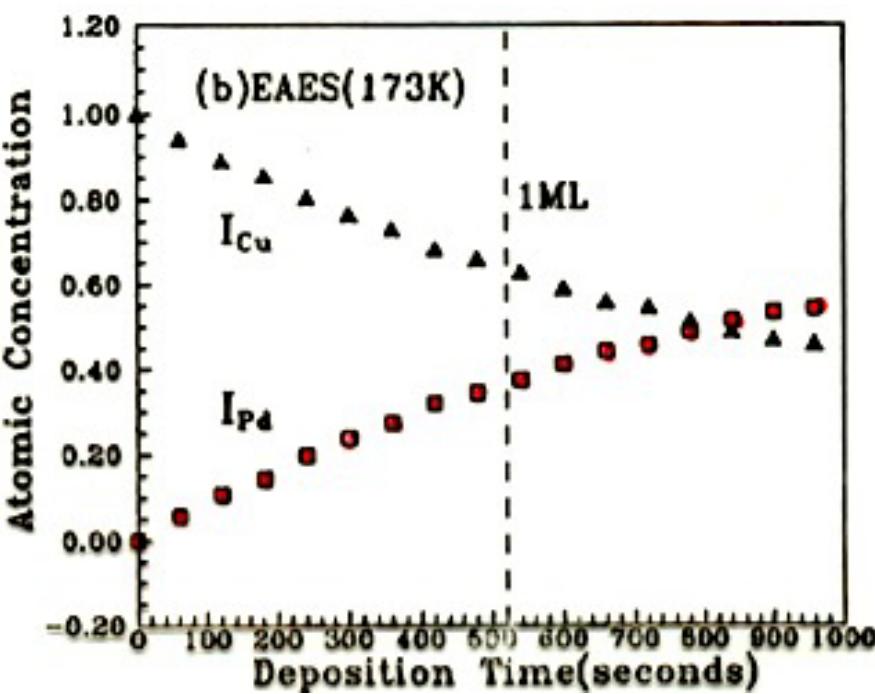
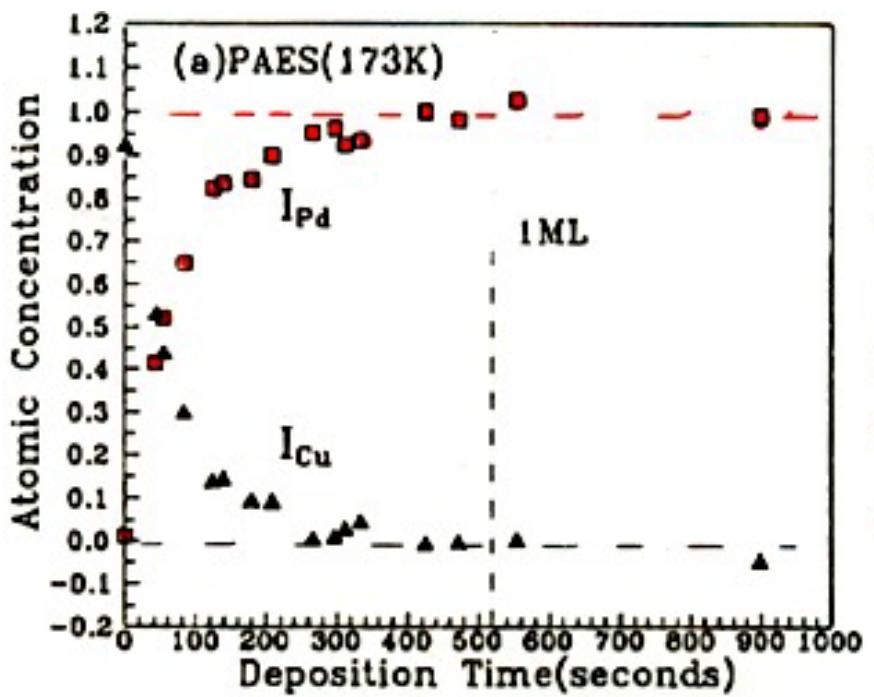
PAES



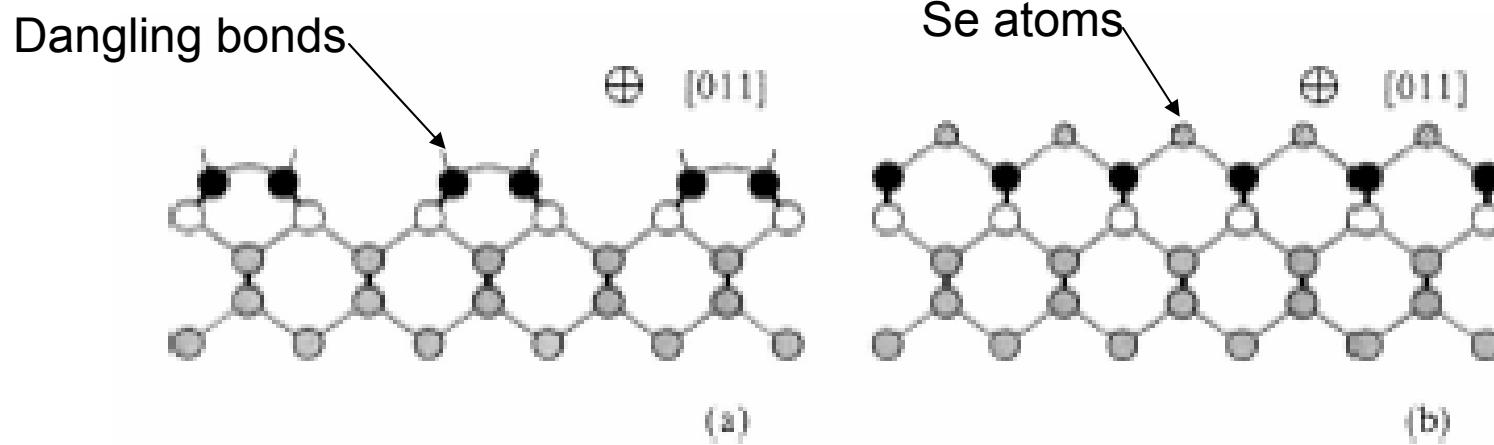
EAES



Cu MVV **Pd NVV** **Cu LVV**



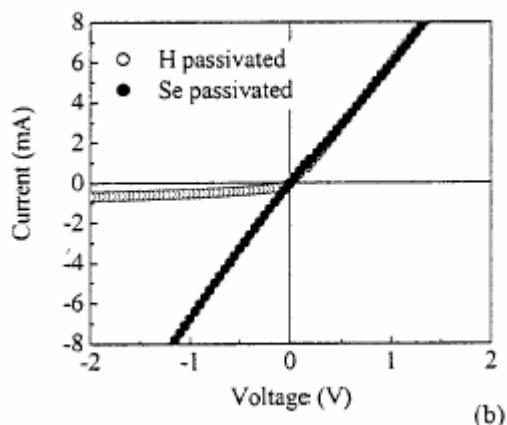
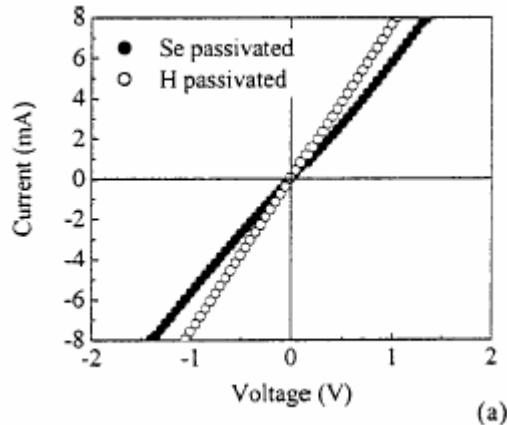
Passivation of Dangling Bonds on the Si(001) surface by Se atoms



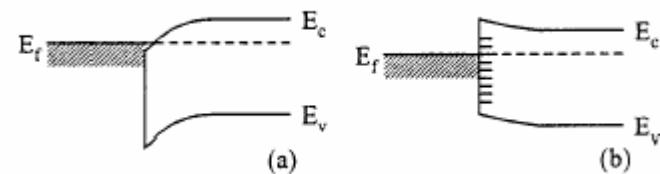
Side view into the [011] direction of (a) the reconstructed Si(001) surface and (b) the Se-passivated Si(001) surface (Tao et al., Appl. Phys. Lett. 2003)

Mg contacts on passivated Si

Passivation prevents formation of Schottky Barrier monolayer of Se more stable than H or S (Tao et al. 2003)



- (a) Ohmic behavior for passivated surfaces
- (b) Diode like I-V curves H passivated surface after annealing – Se surface still ohmic



Interface states caused by mid gap
Fermi-level pinning caused by
interface states from formation of
MgSilicide

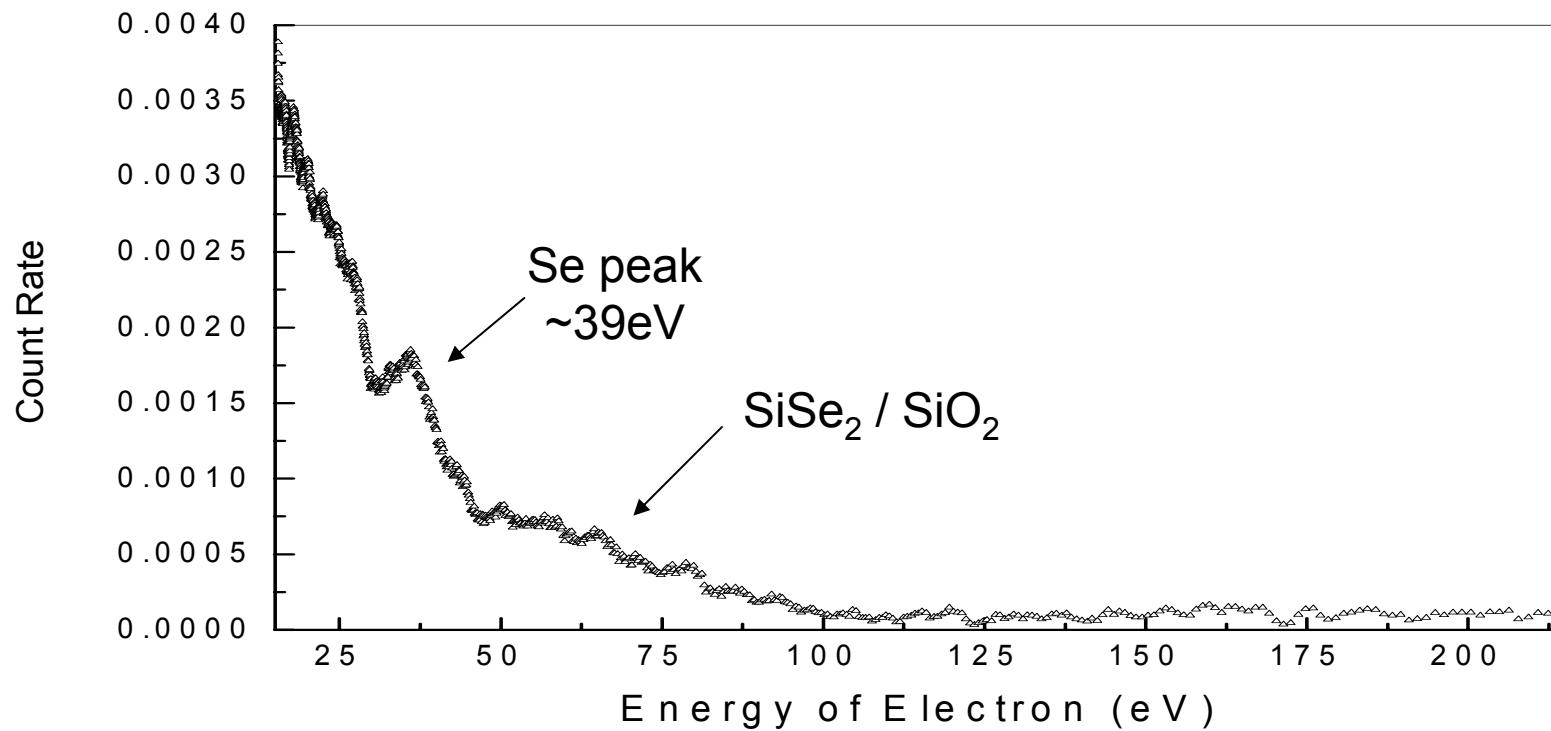
Problem ---- Tao et al. could not show that the monolayer of Se was actually present at the surface before metalization using other analytical techniques

Goal - use surface selectivity of PAES to:

- Prove that Se was still present on Si after removal from MBE system.
- Study the stability of the Se film with respect to atmospheric exposure.
- Study the thermal stability of Se passivation layer.

PAES from Se passivated Si(100) surface

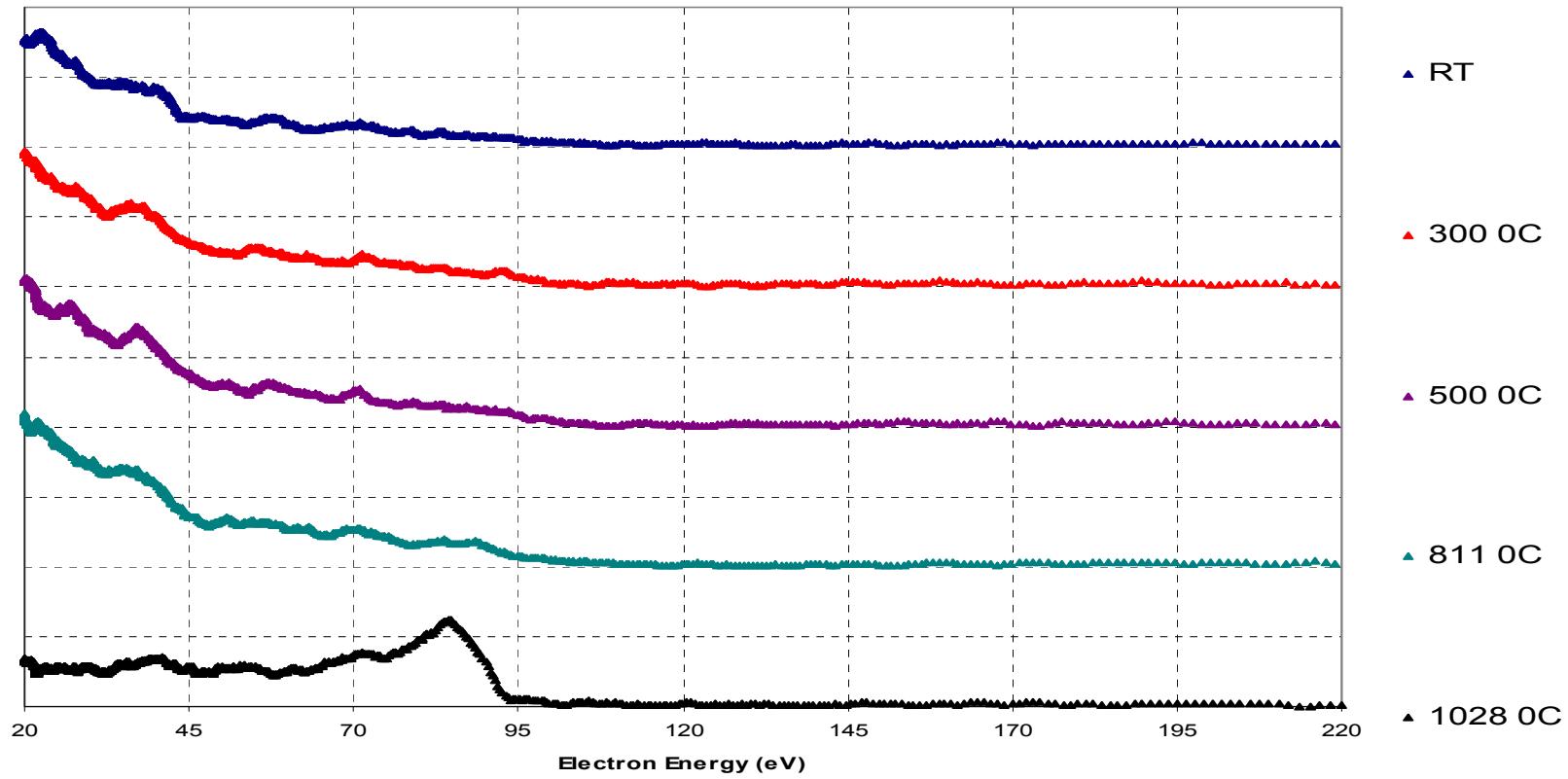
Se(1 ML)/Si(100) sputtering time: 0 hrs, live time: 83389 sec,
e⁺ energy = 15 eV, sample bias = 0 V, TOF tube bias = -17.0 V



Observation:

1. Se_MVV and Si_LVV(SiSe₂ or SiO₂) Auger peaks at ~ 39eV, ~59eV and ~73eV.
2. Se peak is much stronger than Si peaks
3. No pure Si_LVV peak(~89eV) is observed

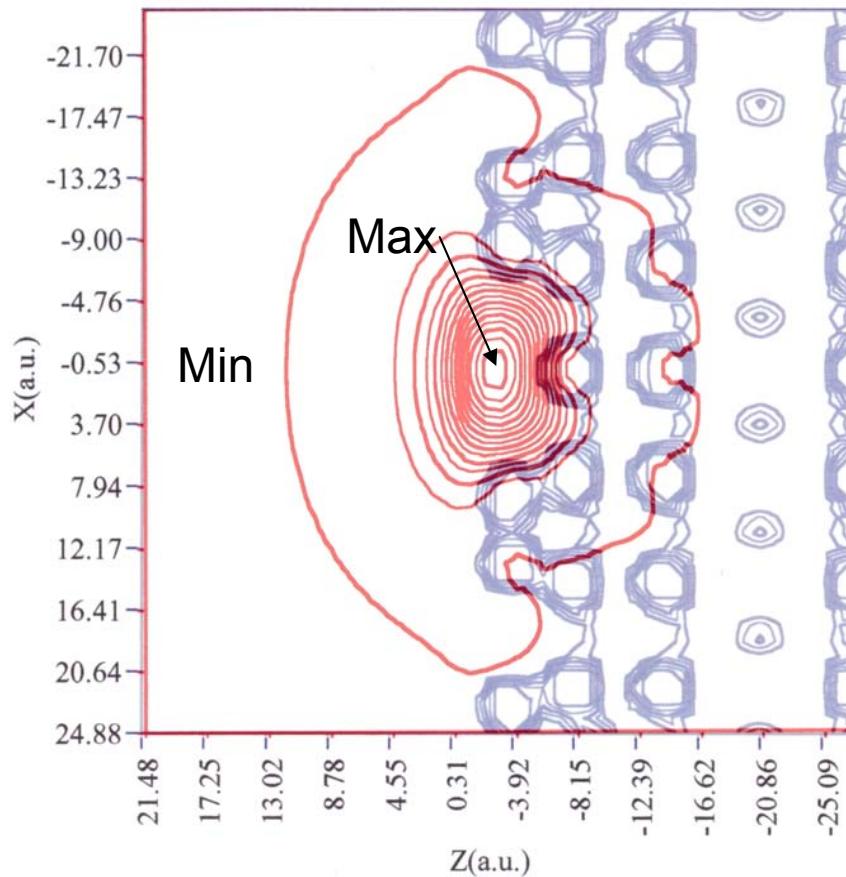
PAES Spectra of Se(1ML)/Si(100) vs. annealing temperatures



Observations

1. Se_MVV and Si_LVV(SiSe_2 or SiO_2) Auger peaks grow with increasing annealing temperature.
2. Pure Si_LVV peak is not observed even at highest annealing temperature.

Sensitivity to Nanostructures on the Surface



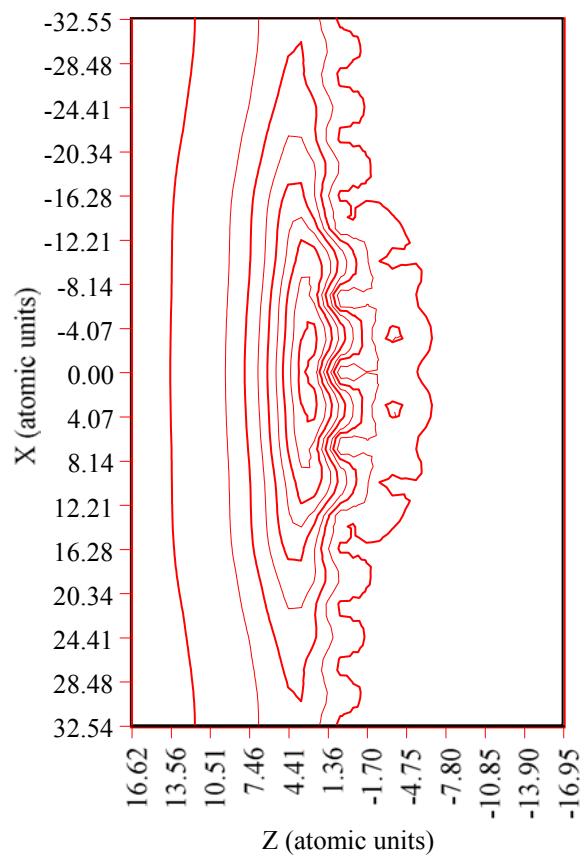
Positron (red contours) trapped in surface “defect*.”
(Potential seen by positron shown in blue).

*Corner-hole in
 $\text{Si}(111)\text{-}7\times 7$ surface

Fazleev et al.

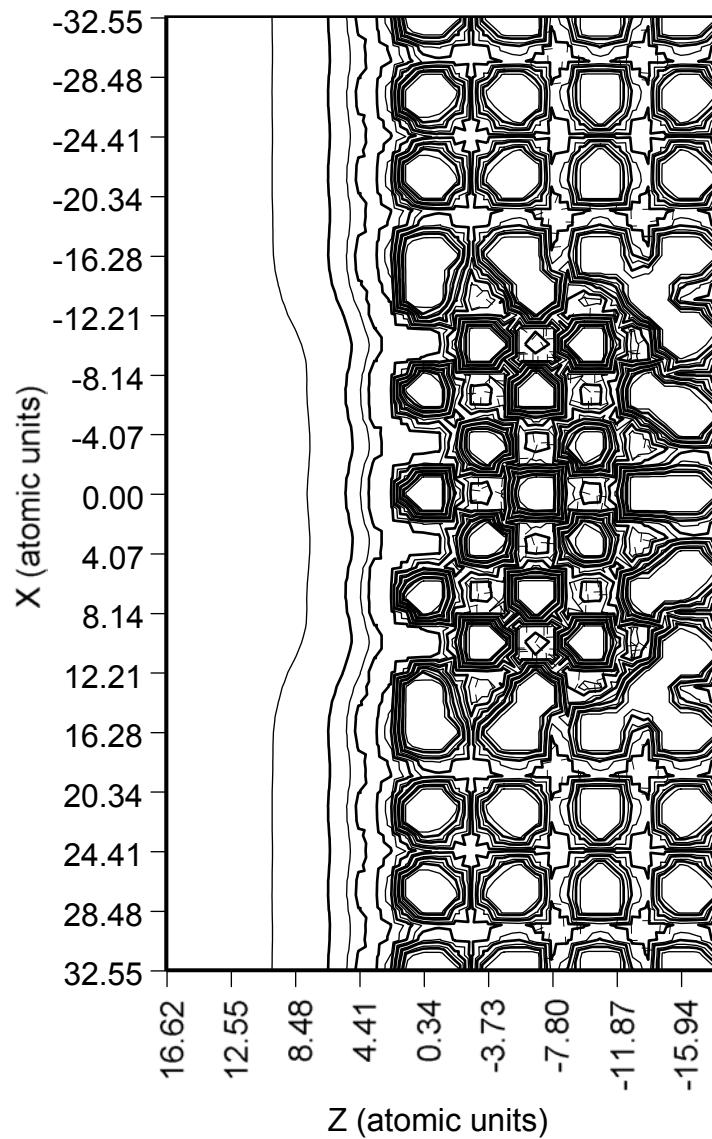
Fe(100) surface with Cu nanoparticle

Vacuum

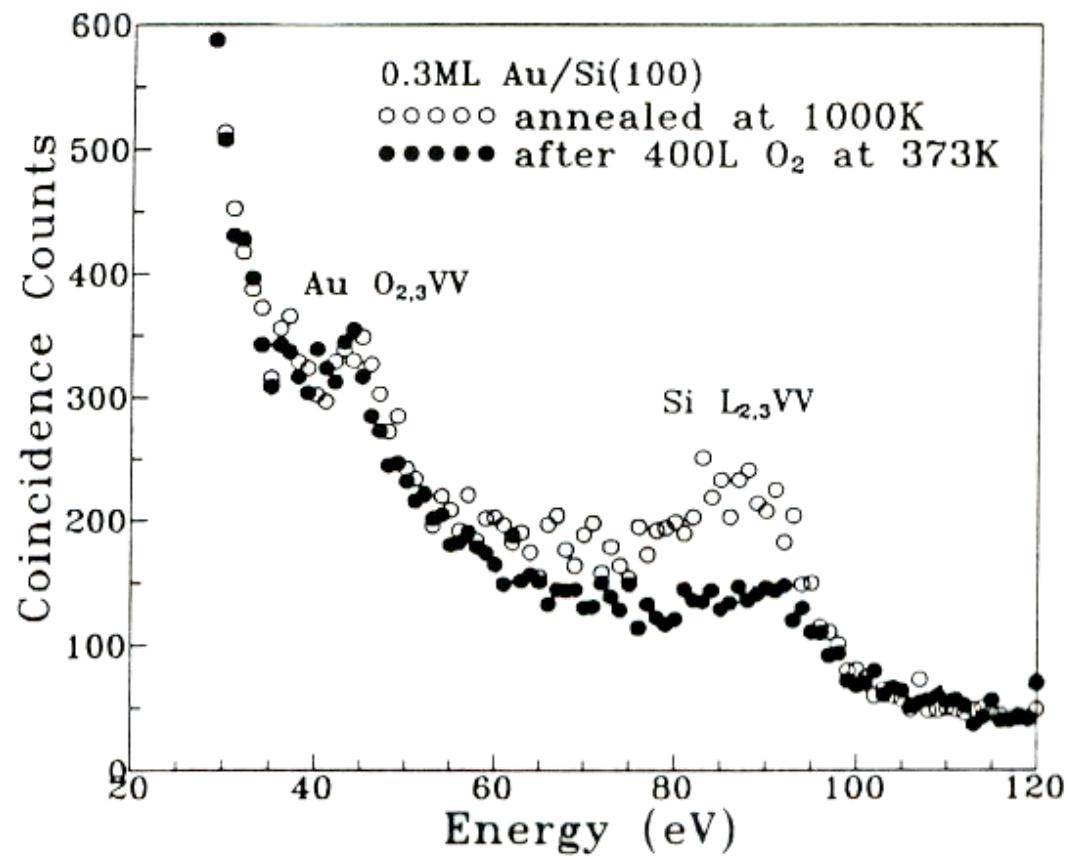


Bulk

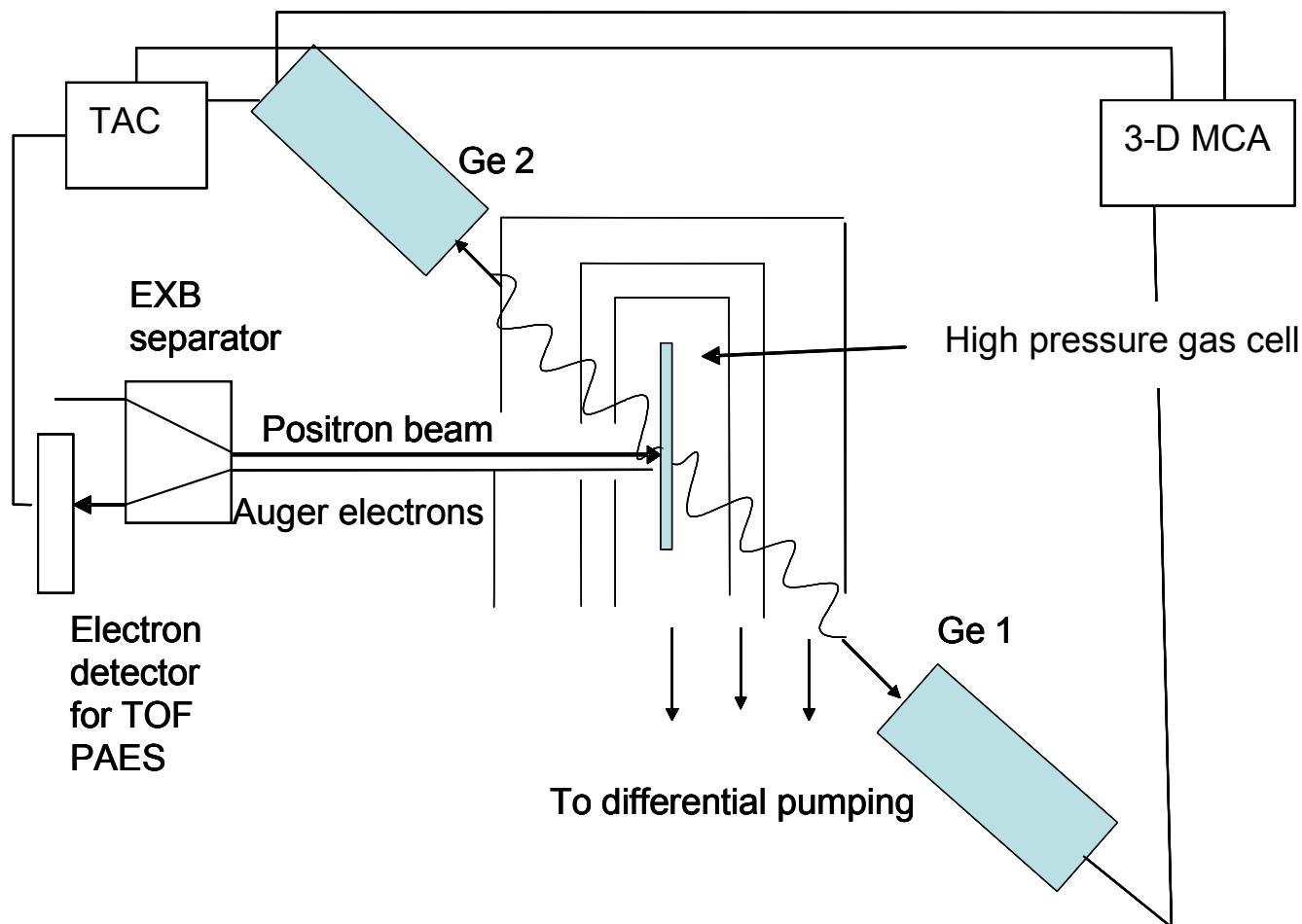
Contour plot of positron surface state
wave function for $Y=0$ at the Fe(100)
surface with Cu nanoparticle



Contour plot of positron potential for $Y=0$ at the



Operando Positron Annihilation induced Gamma Spectroscopy



- Study Chemistry of Gas Solid Interface under Realistic Conditions
- Could be used inside a chemical reactor

Fairy Godmother List

- Intense Positron Beams for Materials Studies (Factor of 10)
- Positron Microscope (Defect Contrast)
- High speed PAES systems for surface studies of thin films, nano-structures, surface defects
- Super (Spin Polarized) ACAR for studying band structure-Fermi surfaces of thin films, magnetic systems, and nano-particles

Acknowledgments:

Current Students:

1. Manori Nadesalingam, 2. Rajalakshmi Sundaramoorthy, 3. Ameena

Undergraduate Students: Brian Davis, Alfonso Hinojosa

Former Students:

M. Jibaly, D. Mehl, C. Lei, L.-W. Tyan, K.-H. Lee, G. Yang, H. Zhou, E. Jung, S. Wheeler, A. Nangia, R. Venkataraman, J.-H. Kim, W.C. Chen, R. Nyak, S. Xie, N. Jian, J. Yan, J. Zhu, S. Kim.

Collaborators (UTA): A. R. Koymen, J.L. Fry, N. Fazleev, C. Kim, A. White, (Japan): Hasegawa, Nagai, (Germany): G. Brauer, S. Hulbert, R. Bartynski

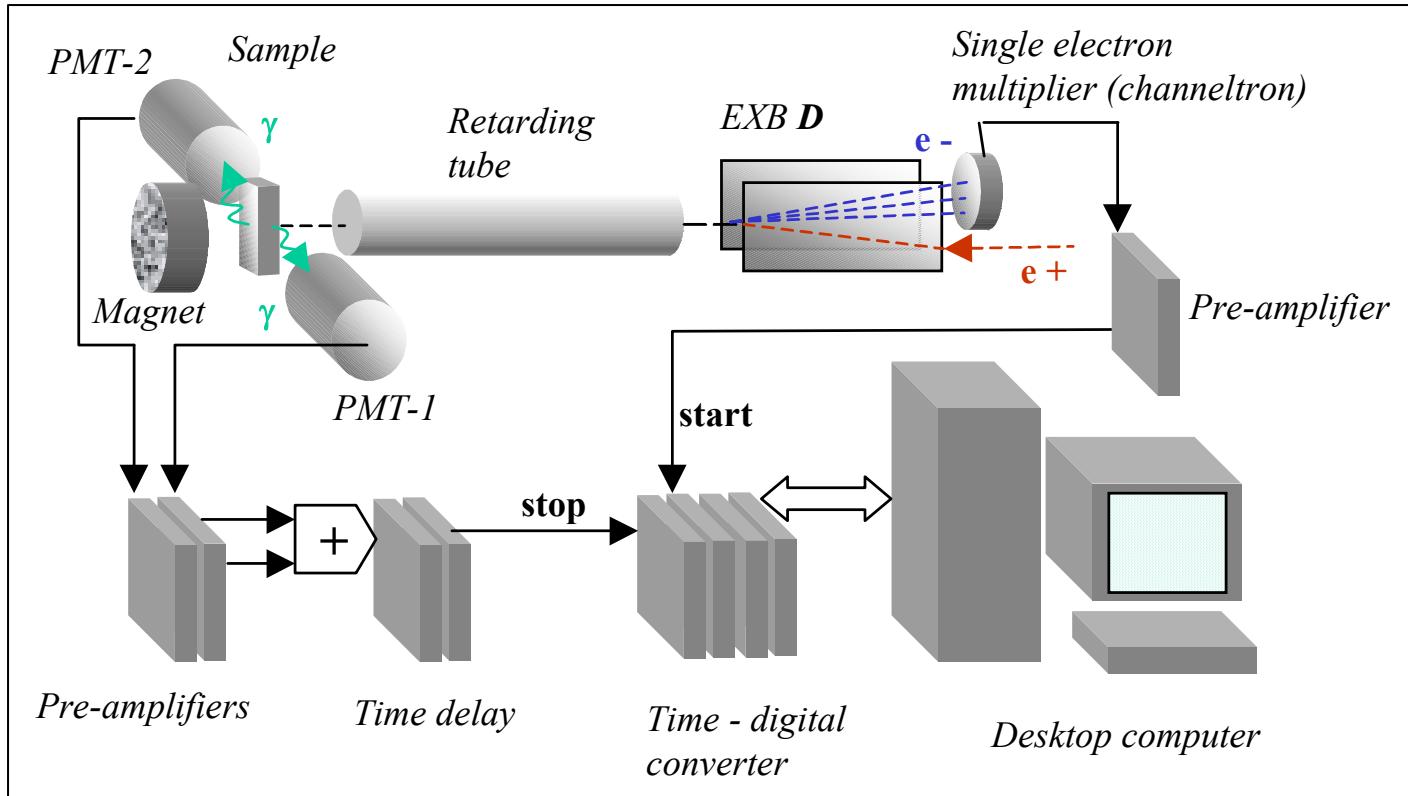
Former Post-Docs/Collaborators: J. Kaiser – UTA, K.O. Jensen - U. of East Anglia, U.K., G. A. Mulholland - SLAC

Rulon Mayer, Arnum Schwab – BNL, Anat Eshed - MIT

Research Sponsored by:

NSF DMR-9812628

The Welch Foundation

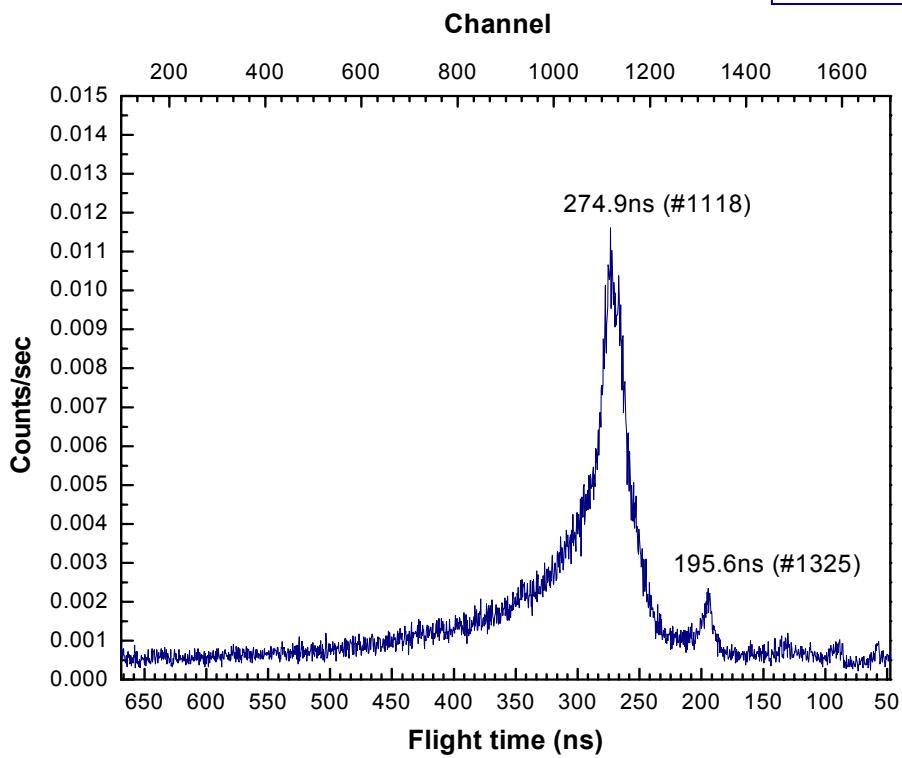


Timing scheme of the Time-Of-Flight PAES spectrometer. The energy distribution of secondary electrons in the TOF technique can be calculated by the equation:

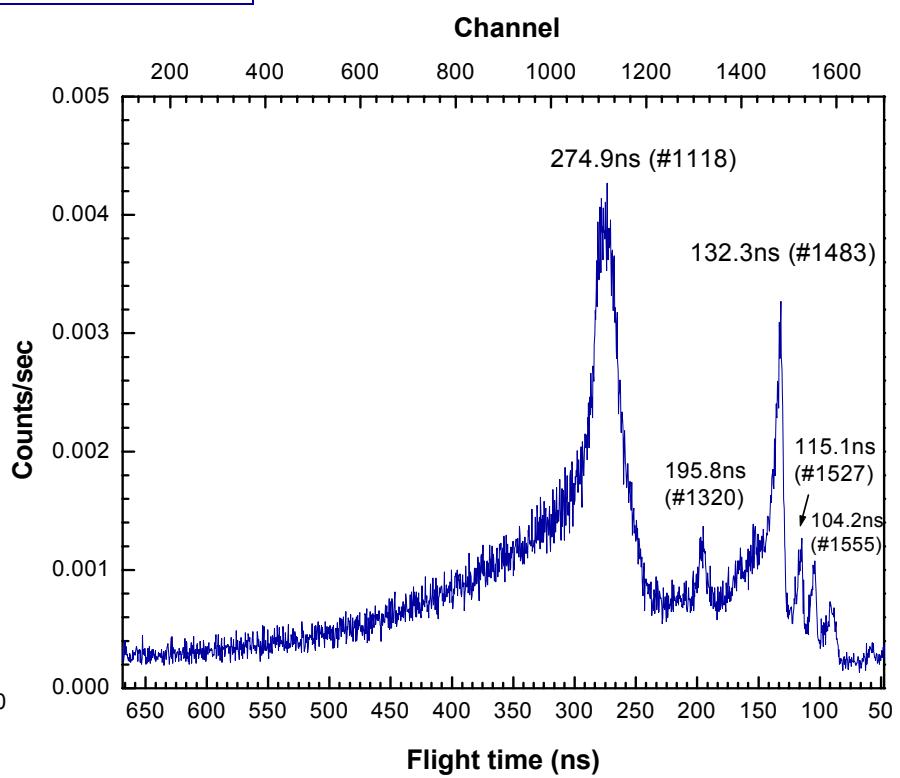
$$E_{kinetic} = \frac{m_e L^2}{2(t_{stop} - t_{start})^2}$$

TOF-PAES Flight Time Spectrum

Copper Sample



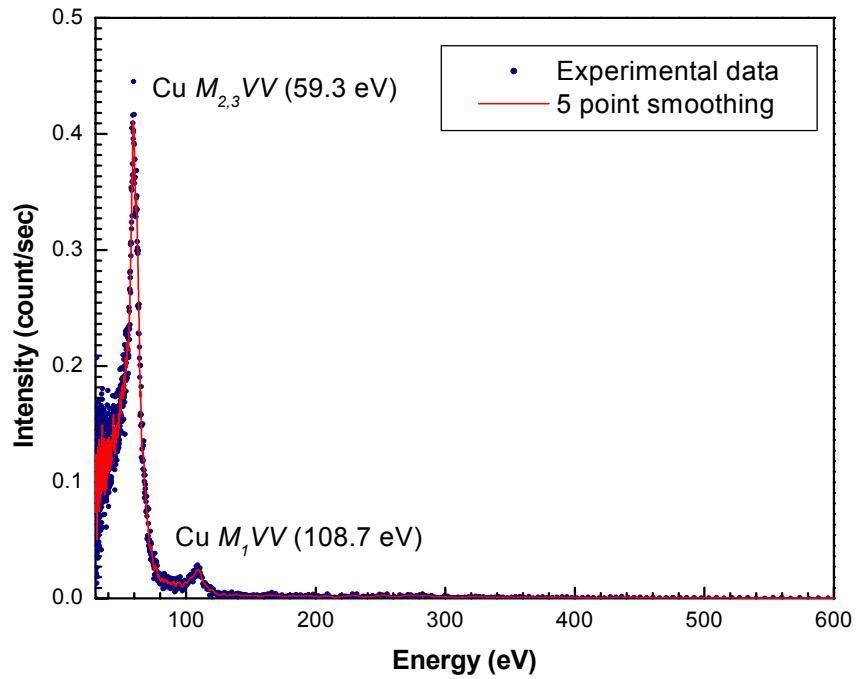
Clean Cu Surface



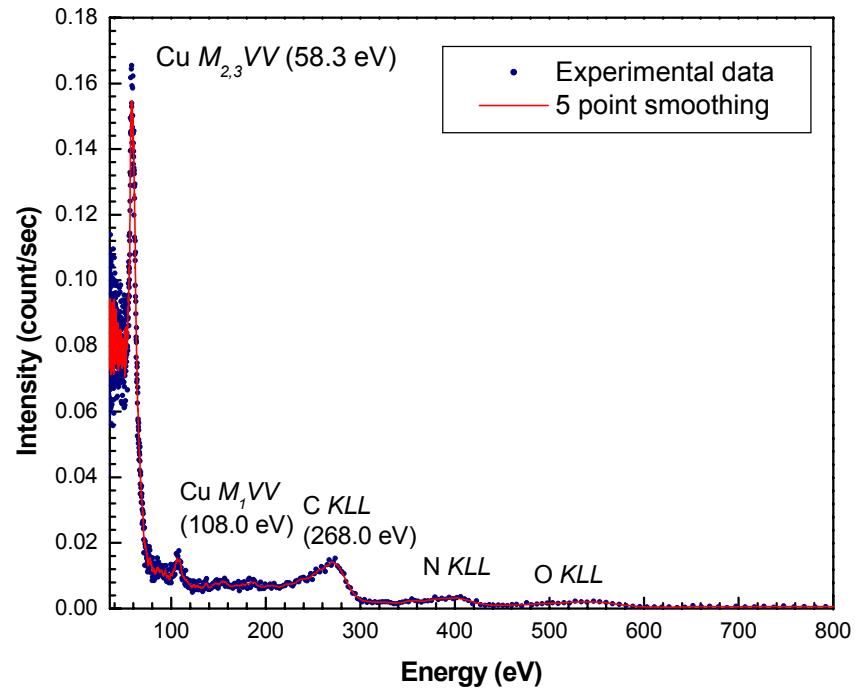
Cu Surface with adsorbates

Flight time spectrum of PAES of Cu surface and corresponding channel numbers.

Energy Spectrum (from T-O-F distribution)



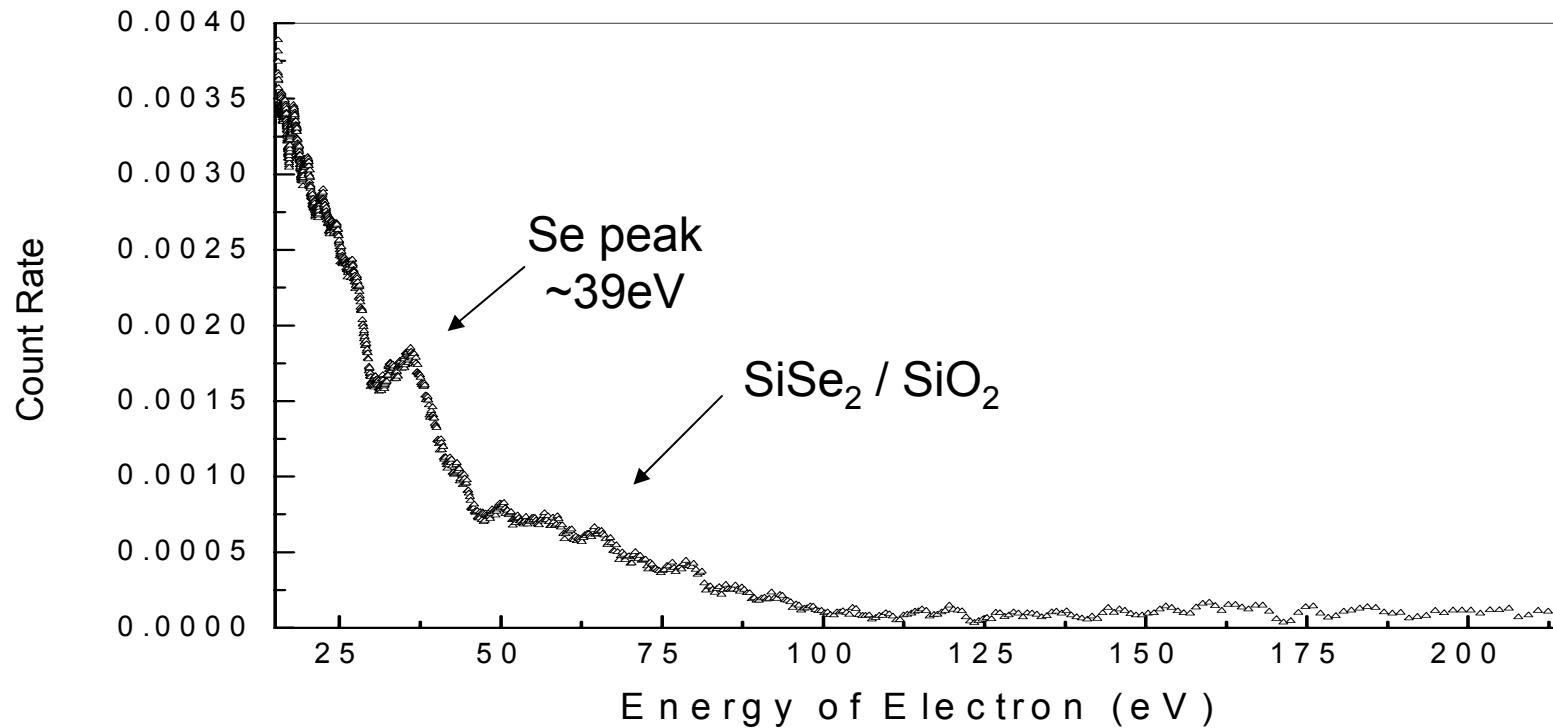
Clean Cu Surface



Cu Surface with adsorbates

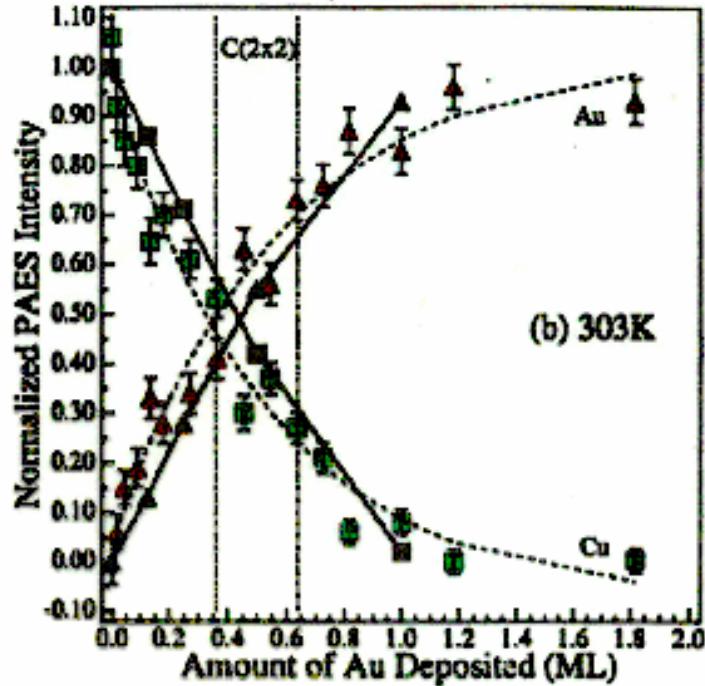
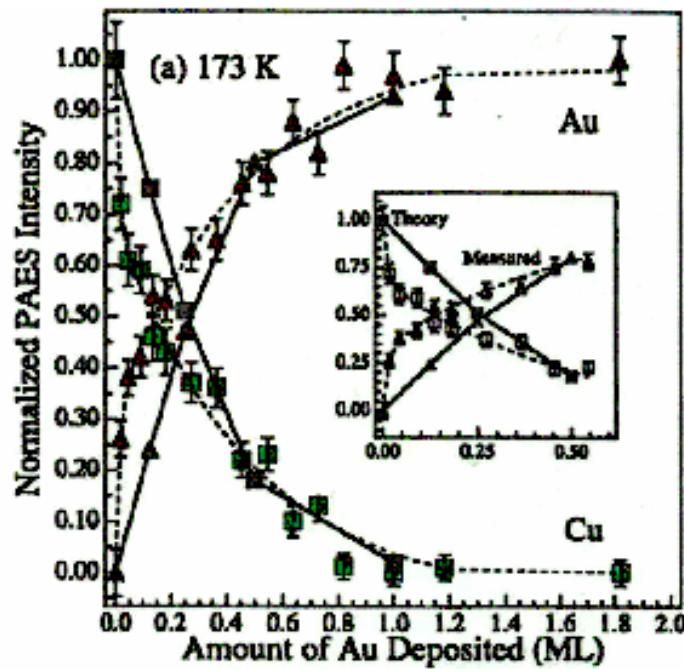
PAES from Se passivated Si(100) surface

Se(1 ML)/Si(100) sputtering time: 0 hrs, live time: 83389 sec,
e+ energy = 15 eV, sample bias = 0 V, TOF tube bias = -17.0 V



Observation:

1. Se_MVV and Si_LVV(SiSe₂ or SiO₂) Auger peaks at ~ 39eV, ~59eV and ~73eV.
2. Se peak is much stronger than Si peaks
3. No pure Si_LVV peak(~89eV) is observed

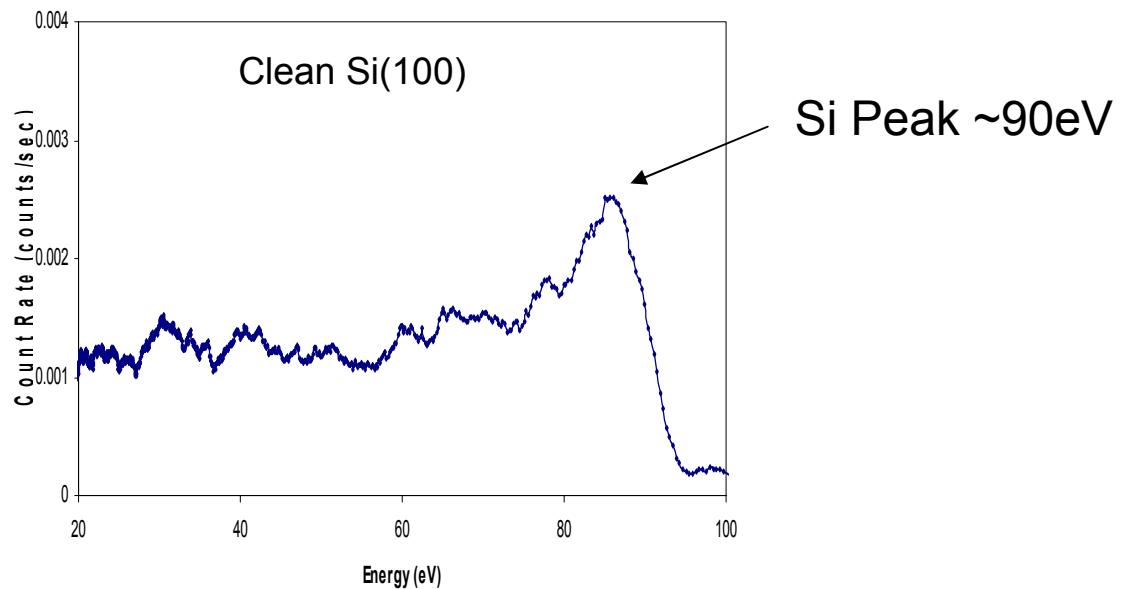
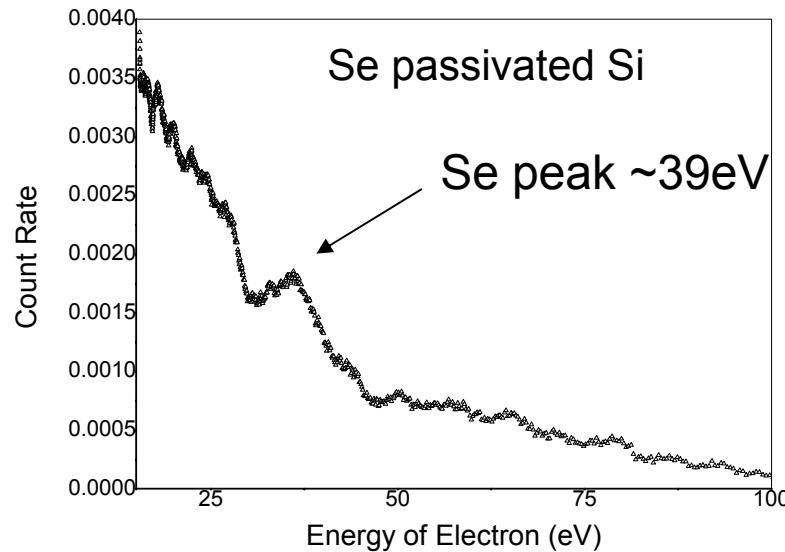


PAES intensity vs. coverage highly non-linear

40% annihilation with Au when surface coverage Au is only 5%!

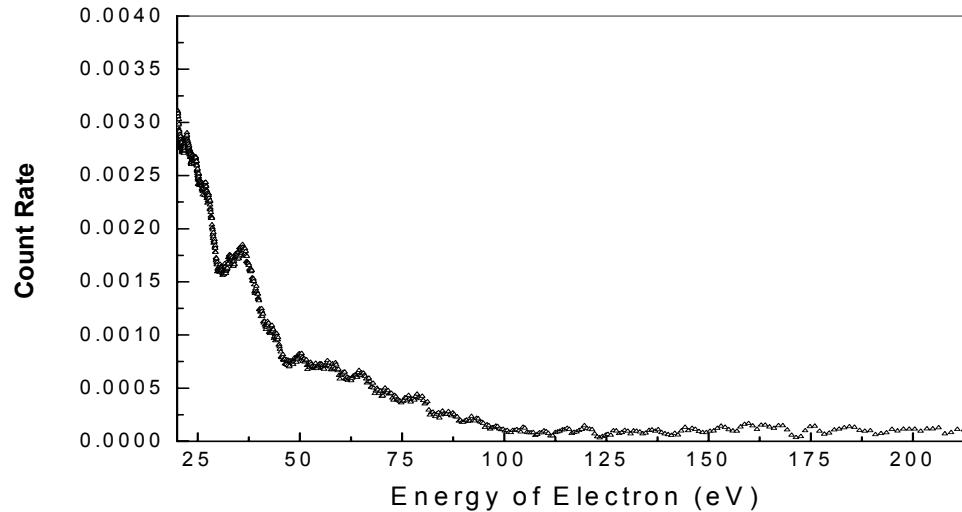
K.H.Lee, G.Vang, A.R.Koymen, Jenson & A.H.Weiss, PRL 72,1866(1994)

Comparison of Se passivated Si with Clean Si reference sample



Comparison of 1-ML Se on Si sample with pure Se reference

sputtering time:0 hrs, livetime: 83389sec,
e+ energy = 15 eV, sample bias = 0 V, TOF tube bias = -17.0V



sputtering time: 2:00 hrs, livetime: 198195sec,
e+ energy = 15 eV, sample bias = 0 V, TOF tube bias = -17.0V

